INVESTIGATIONS OF THE INTERACTIONS OF RADIATION WITH MATTER

FINAL REPORT

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Work on the interaction of radiation with matter is described. In particular charged particle impact ionization of atoms and molecules is discussed, along with photoabsorption by excited states and ground stat atoms, and atomic ions.

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During the period of this contract from the U.S. Army Research Office, our theoretical research in atomic and molecular physics has proceeded apace. In this report, our major areas of investigation are discussed with the progress made in each area highlighted. The results of the calculations provide further insight into the basic nature of these fundamental atomic processes which are of importance as input data for plasma physics, atmospheric, solar, and astrophysics, radiation physics and therapy, for surface studies and catalysis, for studies of the transport of energy from the site of thermonuclear reaction, for energy-loss electron microscopy, for the production of a nuclear-pumped or x-ray laser, for generation and detection of centimeter wavelengths, and for the passage of particle, UV, or x-ray beams through the atmosphere. The report is as non-technical as possible; ample references are given to published works where the technical details can be found. In addition, a complete listing of the 23 publications resulting from this work is presented as an appendix.

I. INTERACTION OF CHARGED PARTICLES WITH MATTER

A major step in this area has dealt with electron ejection in ion-atom collisions where both collision partners have electrons. As a prototype, we have considered He^+ + He collisions[1], since experimental data was available, and we were able to predict the total ejected electron energy (and angular) distribution rather well. The calculation considered electron ejection by both target <u>and</u> projectile so that we were able to delineate which part of the electron distribution came from the target and which came from the projectile; this was not yet available experimentally since the breakdown required a coincidence experiment. From this work, we also learned the importance of the ejection of an electron by one particle and the simultaneous excitation or ionization of the other. Stimulated by these results, a coincidence measurement was made and compared with our calculations.[2] This comparison showed that simultaneous ionization was indeed important, even more important than the calculation predicted, and was the dominant process in certain regions of angle and energy.

We have also made considerable progress in the semi-empirical modelling of electron ejection (δ-ray) cross sections in ion (electron)-atom (molecule) collisions with a view to extending existing data. The model is based generally on the Bethe expansion of the cross section at high impact energies.[3] The leading term in this expansion is related to the photoionization cross section for which there exists significantly more reliable experimental data than for electron ejection cross sections. In the past, have had substantial success applying this technique to protons on atoms,[4] protons on molecules[5], electrons on atoms[4,6] and electrons on molecules.[7] In this work, we have succeeded in using proton data to predict electron impact results. In particular, our predictions for electron impact ionization of water molecules did not agree very well with experiment[8] investigations of the matter convinced us that the experiment had to be in error; a remeasurement has brought experiment and our result into quite good agreement.[9]

In another area we have continued a project, in collaboration with an experimental group, aimed at delineation of the cross sections for the various "ionization pathways" which lead to multiple ionization in ion-atom collisions. By judicious use of extant experimental and theoretical results, we have been able, in some cases, to unravel the picture and extract cross sections of unmeasured processes. Our previous work on the lighter noble gases has been extended to Xe[10] where there is far less data and multiple ionization dominates. Oddly enough, our theoretical predictions are quite good for double and triple ionization but about 50% high for single ionization. This is unexplained, at present.

II. INTERACTION OF ELECTROMAGNETIC RADIATION WITH MATTER

In the area of relativistic effects our primary goal has been to understand in what ways the non-relativistic photoabsorption results are modified by relativistic interactions and to ascertain the underlying cause(s) of these modifications. Owing to the paucity of experimental results, we have been unable to compare our predictions base on simple relativistic calculations with measurements. Thus, to provide some check, we have performed a number of calculations at the sophisticated relativistic-random-phase approximation (RRPA) level.[11] It has been predicted, for example, that the zeroes in the dipole matrix elements, generally referred to as Cooper minima,[12,13,14] each of which break up into three zeroes relativistically, exhibits anomalously large energy splittings among the relativistic zeroes.[15] Our RRPA calculation applied to Rn(Z=86) has found the same result;[16] the splitting in the 6p zeroes are almost exactly the same as in the simple Dirac-Slater (DS) central-field calculation. This is important since the existence and vocation of these "Cooper minima" make a major effect upon the cross section both quantitatively and qualitatively.

We have also applied the RRPA to Yb(Z=70)[17] and found that resulting cross sections were in good agreement the shape of the experimental cross section; the measured values were relative so comparison of absolute cross sections were not possible. Of particular interest, in this case, was the interchannel coupling which modified the 4f cross section at threshold by about a factor of two.

An interesting feature is predicted to occur in the 3p cross section in Kr(Z=36) in both the simple Hartree-Slater (HS)[14] as well as in Hartree-Fock(HF) calculations.[18] These cross sections show structures unrelated to Cooper minima or delayed maxima. It has been suggested that these structures were artifacts of the HS and HF calculations.[19] Since there is no experiment in the region we have performed RRPA calculations to check on this structure.[20] These calculation do indeed show the structure, indicating that it is <u>not</u> a theoretical artifact. Furthermore, good agreement with experiment is found where experiment exists at higher energies, indicating that the RRPA result is very likely reliable in this case.

For open-shell atoms, we have initiated a program to explore the effects of the open shell(s) on the photoabsorption in the inner shell threshold regions where the multiplet structure induced by the open shell(s) is of greatest importance. Calculations have been performed for the photoionization of B(Z=5),[21,22] the simplest atom with an open p-shell. The results show a remarkable deviation from the statistical branching ratios of the various multiplet channels for both 2s and 1s ionization, a deviation which amounts to about 50% near the thresholds and gradually dying out over approximately a 100 eV range. If open-shell effects are so substantial at such low Z, then they are likely to be even more important at higher Z.

In the area of excited state and ionic photoabsorption, we have completed our study of the systematics of the excited states of the alkali atoms. Using simple HS wave functions we have mapped out the phenomenology for Cs(Z=55),[23] especially the multiple minima [24,25] which dominate the near-threshold cross sections. Since there is no experiment yet, we extended these calculations to discrete-discrete transitions where there is <u>some</u> experiment; there is no <u>a priori</u> reason to believe that the model should be better (or worse) for excitation than for ionization. Rather good agreement overall was found for the discrete-discrete transitions.[23]

In addition, owing to the lack of experimental data for ionic photoabsorption, we have undertaken calculations at the RRPA level to ascertain the accuracy of the simpler calculations. We have looked at Al^+, which is dominated by the 2p absorption, thereby yielding a cross section without much structure.[26] This RRPA result is found to be in remarkably good agreement with the simple HS cross section. We have also looked at K^+, where the cross section is dominated by the 3p subshell which displays a Cooper minimum.[13] In the neighborhood of the minimum, the RRPA and HS cross sections differ very markedly, since each has the minimum at a different energy. Furthermore, the RRPA result is in excellent agreement with a recent K^+ experiment.[27] This experiment allowed us to check a theoretical prediction that inner shell ionization in ions is unaffected by removal of outer shell electrons as a function of photon energy.[28] Although error bars are large comparison of K and K^+ photoabsortion cross sections tended to confirm this prediction.[29]

We have also begun a program to investigate photoabsorption of excited states of ions. Simple arguments indicate that in going from neutral atoms to ions the photoionization cross section should become simpler and more hydrogen-like. However, this transition to simplicity need not be monotonic nor rapid. Preliminary results for the excited nf states of the Cs isoelectronic sequence have shown that simple cross sections for the neutral become far more complicated for Ba^+ owing to f-wave orbital collapse.[30] Going up 10 stages of ionization to Tb^{+10}

still does not give cross sections as simple as the neutral. Thus, it is clear that ions are <u>not</u> necessarily simpler than atoms.

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